LLNL-CONF-425382

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March 11, 2010

14th International Detonation Symposium
Coeur d'Alene, ID, United States
April 11, 2010 through April 16, 2010

A Constitutive Model for Long Time Duration Mechanical Behavior in Insensitive High Explosives

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Abstract. An anisotropic constitutive model for the long term dimensional stability of insensitive high explosives is proposed. Elastic, creep, thermal, and ratchet growth strains are developed. Pressure and temperature effects are considered. The constitutive model is implemented in an implicit finite element code and compared to a variety of experimental data.

Introduction

At Lawrence Livermore National Laboratory (LLNL) there is an interest to better understand the long term dimensional stability of insensitive high explosive (IHE) components. As these components survive past their intended design lifetimes, margins and uncertainties regarding their mechanical performance must be reevaluated. In particular, material models that can handle transient thermal and mechanical loads over long time spans, including creep and stress relaxation phenomena are desired. However, current material models are inadequate to provide a predictive capability. We at LLNL have developed an extensive experimental capability to measure the mechanical behavior of explosives subject to various thermal and mechanical loads. This capability has proven invaluable as we seek to develop and calibrate our material models. In this paper, we develop a constitutive model for IHEs that consist of a triaminotrinitrobenzene (TATB) explosive and a Kel-F binder. This model is based on phenomenological data rather than first principles. We implement this constitutive model in NIKE3D [1], an implicit FEA code, and benchmark its behavior against experimental data. Figure 1 shows cross section of a model of a typical test specimen undergoing creep. Deformations are exaggerated by 15 times in this figure.

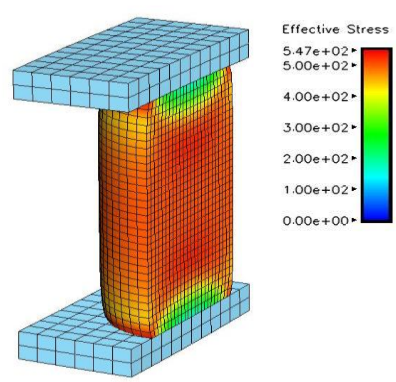

Fig. 1. Typical Creep Compression Test Specimen.

One Dimensional Strains

Over a variety of conditions, a linear relationship between creep strain and the logarithm of time was observed for constant uni-axial loads and fixed temperatures. Figure 2 shows a typical sample of this data for a variety of temperatures (-54 to 70°C) and stresses (250 to 780 psi).

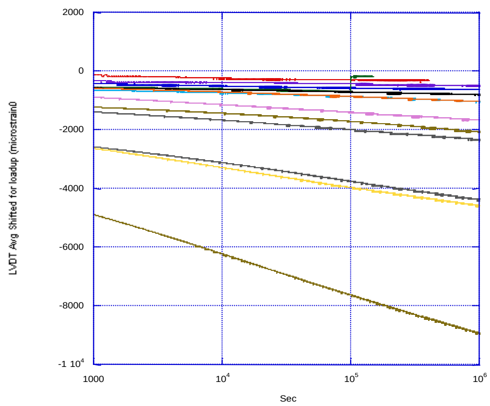

Fig. 2. Creep Strain as Function of Time for a Variety of Uni-axial Stresses and Temperatures.

Preserving this log-linear creep response limits the form the material model can take. In this paper the total strain is decomposed into the following components: elastic strain, recoverable creep (visco-elastic like), non-recoverable creep (damping like), thermal expansion, and ratchet growth. The creep strain is further decomposed into hydrostatic and deviatoric components. Each of the strain components is assumed to respond independently to the applied stress and each is consistent with the observed log-liner behavior.

This log-linear relationship may be expressed in equation form is,

$$\varepsilon = g \log\left(\frac{t}{t^0}\right) \qquad (1)$$

where g is the log slope and is a function of both stress and temperature. The variable t represents the time that the material has been under stress while t^0 represents the time at which the strain in this relationship is zero. Clearly, this relationship is not valid for times less than t^0. Typical values of t^0 are much smaller than one second. Experiments suggest that this relationship is valid from minutes to at least months. We found that t^0 may be assumed to be a function of temperature only. We further found that the coefficient, g, may be accurately deconvolved into a quadratic function of stress multiplied by a function of temperature as shown below,

$$g = ab \qquad (2)$$

$$a = a\ \sigma\ =\ c_1 + c_2\sigma\ \ \sigma \qquad (3)$$

$$b = b\ T \qquad (4)$$

where c_1 and c_2 are constants. The function b, as a function of temperature, is shown in Figure 3. Figure 4 shows the function g as a function of stress for a variety of temperatures. This figure also shows the experimentally measured log-slopes used to calibrate these curves.

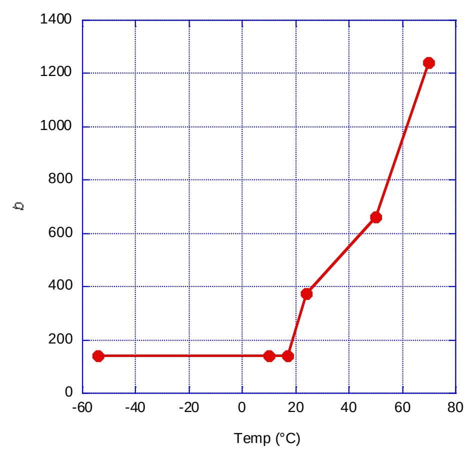

Fig. 3. Temperature Dependent Coefficient,b, of The Log Slope.

One-Dimensional Elastic Strains

The strain is decomposed into elastic and creep components, and the time is offset by t^E, such that creep strain is zero at time zero:

$$\varepsilon = g \log\left(\frac{t^E}{t^0}\right) + g \log\left(\frac{t + t^E}{t^E}\right) \qquad (5)$$

The first term in this equation is the elastic component of strain and the second term is the creep component of strain. For the IHE examined in this paper a time of 20 seconds was found to be appropriate for t^0. Note that t/t^E is large for the time scales of interest. The value of t^E is assumed to be constant. The physical interpretation of this decomposition may be thought of as allowing an initial elastic strain and then immediately picking up the log-linear creep curve staring at the time consistent with that strain. As a result of this assumption, loads of a very short duration result in an effectively elastic response. Figure 5 shows the values of t^0 based on the experimental strain data fit at t^E and the log slope calculated in equation 2.

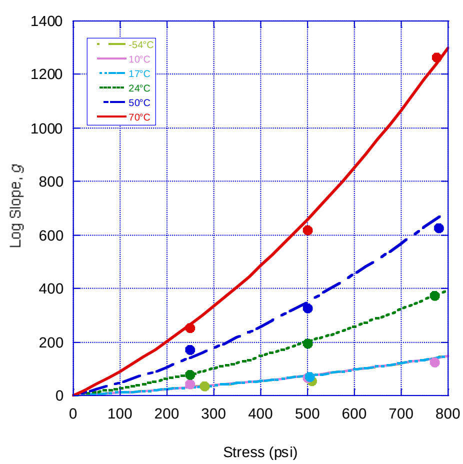

Fig. 4. Log-Slope as a Function of Stress for Various Temperatures.

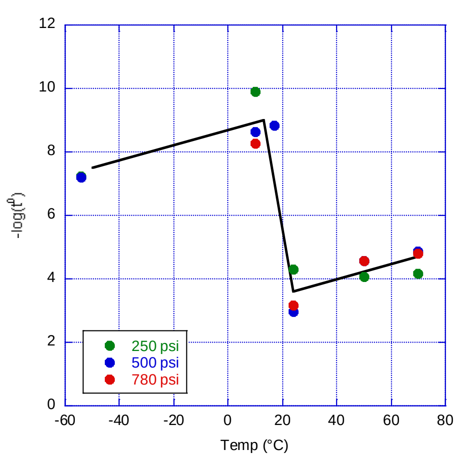

Fig. 5. log t^0 vs. time.

Three-Dimensional Generalization

The one dimensional creep model is generalized to three dimensions by generalizing the function a as follows,

$$a_{ij} = c_1^d + c_1\sigma' \; \bar{C}^d_{ijkl}\sigma_{jk} + c_1^v \bar{C}^d_{ijkl}\sigma_{kl} \tag{6}$$

$$c_1^d + c_1^v = c_1 \tag{7}$$

Where c_1^d and c_1^v are the devitoric and volumetric components of the compliance tenors, respectively. The super bar indicates that the tensor has been normalized by the 1111 value. This normalization is not arbitrary, but corresponds to our one dimensional calibration test data. The coefficient c_1 is split into a deviatoric component, c_1^d, and a volumetric component, c_1^v. The ratio between these two material properties contains the "Poisson's ratio" information that was lost when the compliance tensor was split and normalized. This generalization retains the one dimensional response while allowing for three dimensional and anisotropic behavior. It should be noted that the volumetric response is assumed to be linear with regard to stress. We have limited data to support this assumption.

Elastic Strains

The deviatoric elastic strain ε_{ij}^{Ed} may now be written explicitly as,

$$\varepsilon_{ij}^{Ed} = c_1^d + c_2\sigma' \; \bar{C}^v_{ijkl}\sigma_{kl} \log\left(\frac{t^E}{t^0}\right) \tag{8}$$

Likewise the elastic volumetric strain, ε^{Ev} may be written as,

$$\varepsilon^{Ev} = c_1^v \bar{C}^v_{ijkl}\sigma_{kl} \log\left(\frac{t^E}{t^0}\right) \tag{9}$$

Recoverable Devitoric Creep Strains

The recoverable (visco-elastic like) devitoric creep is modeled with n sets Voigt elements per strain direction. Each Voigt element consists of a spring and dashpot connected in parallel while the Voigt elements are connected in series. The recoverable strain is thus found by summing the internal Voigt strains,

$$\varepsilon_{ij}^{rd} = \sum_{s=1}^{n} \varepsilon_{ijs}^{rd} \tag{10}$$

In order to capture the correct log-slope, the Voigt parameters are found to be functions of stress and temperature. For a given stress and temperature, the Voigt parameters may be found such that, the change in the internal Voigt stains over a time interval are,

$$\varepsilon_{ijs}^{rd} = \delta a_{ij}^{rd} - \varepsilon_{ijs}^{rd} \quad 1-e^{-\omega_s^{rd}\Delta t} \tag{11}$$

where

$$\omega_s^{rd} = \omega_0 \left(\frac{\delta e}{b}\right)^s \tag{12}$$

$$a_{ij}^{rd} = c_1^d + c_2 \sigma' \quad \bar{C}_{ijkl}^d \sigma_{jk} \tag{13}$$

where δ is a parameter that scales the spacing of the characteristic response times. This selection of Voigt parameters ensures the correct average log-slope and that the characteristic response times are functions of temperature only. The long term equilibrium strains are functions of stress only. The average log-slope is not a function of δ, however, the smaller δ/b is, the smoother the response curve will be, and the higher n will need to be for the response to be valid over the time scale of interest. The value of ω_s is set to ensure that the log linear fit for a given δ/b crosses zero strain at t^E (20 sec). Figure 6 shows a typical creep response for a δ/b of 2 and 6, and an n of 12 and 4, respectively.

The linear range in this figure is from 10's of seconds to hundreds of years. Note that a δ/b of 6 is too large and the response significantly deviates from linear.

Recoverable Volumetric Creep Strains

The recoverable (visco-elastic like) volumetric creep is modeled in a similar fashion,

$$\varepsilon^{rv} = \sum_{s=1}^{n} \varepsilon_s^{rv} \tag{14}$$

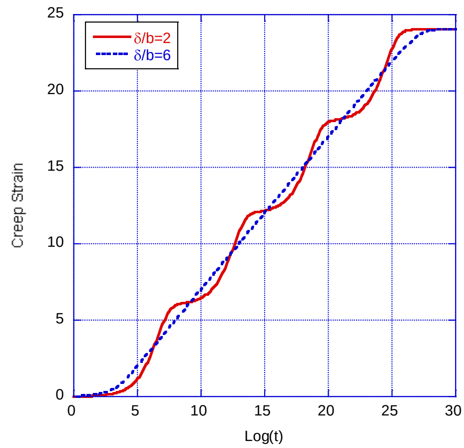

Fig. 6. Log-Linear Respons of Recoverable Creep.

where ε^{rv} is the recoverable volumetric strain. This volumetric strain likewise evolve over a time interval as follows,

$$\Delta\varepsilon_s^{rv} = \delta a^{rv} - \varepsilon_s^{rv} \quad 1-e^{-\omega_s^{rv}\Delta t} \tag{15}$$

$$\omega_s^{rv} = \omega_0 \left(\frac{e\delta}{b}\right)^s \tag{16}$$

$$a^{rv} = c_1^v \bar{C}_{ijkl}^v \sigma_{jk} \tag{17}$$

Non-recoverable Devitoric Creep Strains

Non-recoverable creep strains are the components of the creep strain that will not recover to its original state without an external load. The non-recoverable devitoric creep strains are modeled essentially as damping that increases as the material is worked. An 'effective creep surface' similar to a yield surface is conceived. Thus, depending on the direction of creep, the perceived creep that has already occurred will differ, and therefore so will the current creep rate. Figure 7 shows a two dimensional representation of this surface.

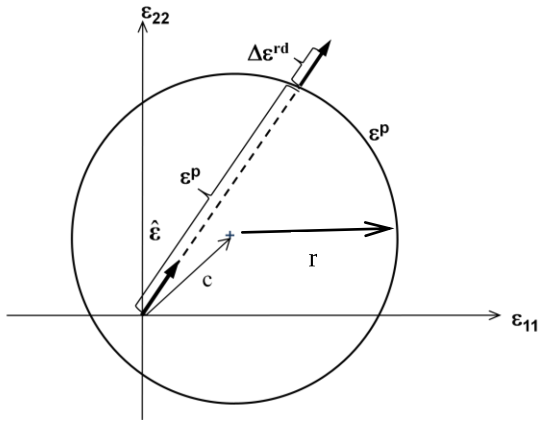

Fig. 7. Two-Dimensional Representation of Effective Creep Surface.

The flow direction of the non-recoverable devitoric creep is defined by the unit tensor,

$$\hat{\varepsilon}_{ij} = \frac{q_{ij}}{\left(q_{kl} q_{kl}\right)^{1/2}} \tag{18}$$

$$q_{ij} = C^{d}_{ijkl}\sigma_{kl} \tag{19}$$

For a "spherical" effective creep surface the perceived creep strain magnitude, or the distance in tensor space from the origin to the effective creep surface, can be shown to be,

$$\varepsilon^{p} = \gamma + \left(\gamma^{2} + r^{2} - c_{ij}c_{ij}\right)^{1/2} \tag{20}$$

$$\gamma = \hat{\varepsilon}_{ij}c_{ij} \tag{21}$$

where c_{ij} represents the location of the center of the surface in strain space and the radius, r. Using the one dimensional log-linear creep relationship in equation 5, a perceived time, t^{p}, may be calculated as a function of the perceived creep strain magnitude,

$$t^{p} = t^{E}\left(e^{\frac{\varepsilon^{p}}{a^{nd}b}} - 1\right) \tag{22}$$

$$a^{nd} = \left(c_{1}^{d} + c_{2}\sigma'\right)\left(\bar{C}^{d}_{ij11}\bar{C}^{d}_{ij11}\right)^{1/2} \tag{23}$$

Note that the stress dependent log slope coefficient "a" is scaled to account for the fact that it was originally normalized to calculated the log slope of ε_{11}, but this formulation utilizes the magnitude of the full strain tensor. Base on this perceived time, the one dimensional log-linear response, and the direction of creep, the change in the non-recoverable devitoric creep strain over a time increment is be found to be,

$$\Delta\varepsilon^{nd}_{ij} = a^{nd}b\log\left(\frac{t^{p} + \Delta t}{t^{p}}\right)\hat{\varepsilon}_{ij} \tag{24}$$

The evolution of the surface is determined by the kinematic damping parameter κ,

$$\Delta c_{ij} = \kappa\Delta\varepsilon^{nd}_{ij} \tag{25}$$

This parameter determines how much the center of the surface is 'dragged' versus expanded. When κ is zero, the surface center remains at the origin. For monotonic loading κ does not affect the material behavior. In order to remain on the surface, the radius of the surface must evolve as follows,

$$\Delta r = \left|\varepsilon^{p}\hat{\varepsilon}_{ij} + \Delta\hat{\varepsilon}_{ij} - c_{ij} - \Delta c_{ij}\right| - r \tag{26}$$

This formulation ensures that, if the stress and temperature remain constant over a period of time, then the creep strain obtained will not be dependent on time the step size.

Non-recoverable Volumetric Creep Strains

The non-recoverable volumetric strain is calculated in a similar fashion the recoverable devitoric strain. The perceived strain is found to be,

$$\varepsilon^{p} = c + r\theta \tag{27}$$

$$\theta = \frac{\sigma_{ii}}{\left|\sigma_{ii}\right|} \tag{28}$$

where θ is the direction of volumetric creep. The perceived time may be similarly calculated as,

$$t^{p} = t^{E}\left(e^{\frac{\varepsilon^{p}}{a^{nv}b}} - 1\right) \tag{29}$$

$$a^{nv} = c_{1}^{v}\bar{C}^{v}_{ijkl}\sigma_{jk} \tag{30}$$

And the non-recoverable volumetric creep strain and state variables likewise evolve over a time interval as follows,

$$\Delta\varepsilon^{nv} = a^{nv}b\log\left(\frac{t^{p} + \Delta t}{t^{p}}\right)\theta \tag{31}$$

$$\Delta c = \kappa \Delta \varepsilon^{nv} \tag{32}$$

$$\Delta r = \left| \varepsilon^{p} + \Delta \varepsilon^{nv} - c - \Delta c \right| - r \tag{33}$$

Confining Pressure

We found experimentally that increasing the confining pressure slows the devitoric creep strain in uni-axial compression tests more than the reduction in von Mieses stress would otherwise predict. We assume an equivalence between the stress state and the temperature to account for this effect. To capture this effect $\tilde{b}$ is substituted for b in the devitoric creep formulations. To calculate $\tilde{b}$, b is scaled by λ,

$$\tilde{b} = \lambda b \tag{34}$$

Figure 8 shows the function λ as a function of $\sigma_{ii} + \sigma'$.

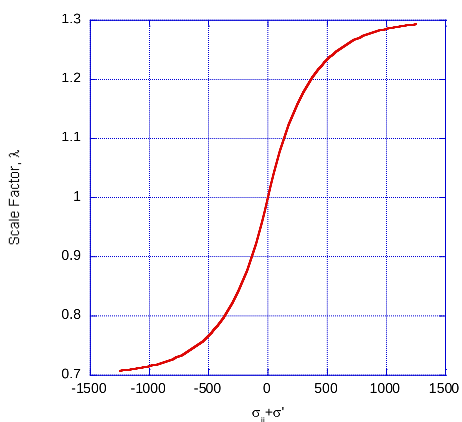

Fig. 8. λ as a function of $\sigma_{ii} + \sigma'$.

This formulation provides a better fit to available data than if lambda was a function of σ_{ii} alone. Note that for uni-axial compression with no confining pressure λ equals one. The right half of Figure 8 is largely speculation.

Figure 9 and Figure 10 show a comparison between the modeled and experimentally determined values of the log-slope for a number of temperatures, axial compressive stresses, and confining pressures. Each line on the graph represents a given axial stress and temperature. The abscissa of the graph is the Tresca stress, which in this case is the axial compressive stress subtracted from the confining pressure. The left side of the graph represents hydrostatic loading, while the terminus of each line represents the unconfined axial loading condition.

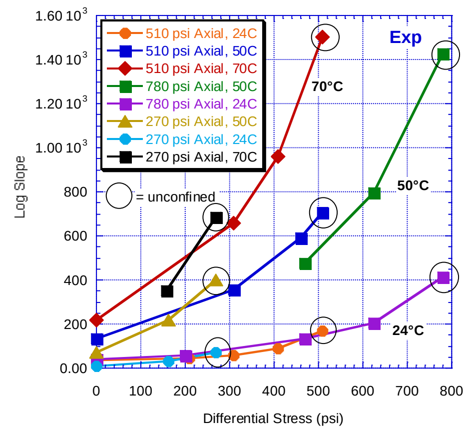

Fig. 9. Experimentally Measured Log-Slope

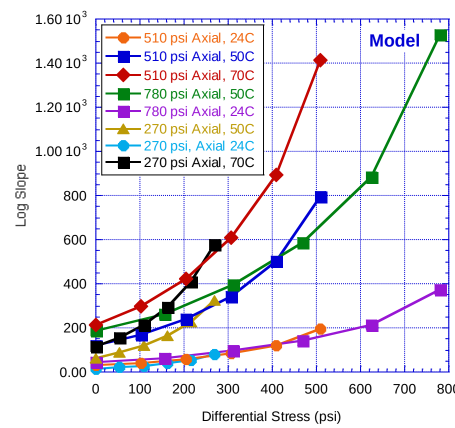

Fig. 10. Model prediction of the Log-Slope.

It should be noted that the function λ and constant c_1 were calibrated using this data.

Thermal strains

The thermal strains are typically anisotropic in IHE's. This anisotropy is dependent on the pressing environment and is assumed to remain constant throughout the material's life. The magnitude of the thermal strains is assumed to be a non-linear function of temperature and is modeled as,

$$\varepsilon_{ij}^{therm} = \bar{\alpha}_{ij}[\alpha(T - T^{ref})] \qquad (35)$$

Where $\bar{\alpha}_{ij}$ represents the thermal anisotropy tensor, α secant coefficient of thermal expansion, and T and T^{ref} are the temperature and reference temperature respectively. The value $\bar{\alpha}_{ii}$ must be equal to one, in order for it not to change the volumetric thermal strain.

Ratchet Growth Strains

Ratchet growth is a phenomenon where cycling the temperature (above a threshold, T^{crit}) causes a permanent increase in volume. We assume that each temperature range cycled through has an asymptotically approached maximum ratchet strain associated with it. Experiments have shown that the ratchet growth effect is enhanced if there is a cold cycle (below a threshold, T^{cut}) before a hot cycle and that ratchet growth is suppressed by pressure. The volumetric ratchet growth, $\varepsilon^{\mathrm{rat}}$, is calculated by integrating the ratchet growth associated will each differential temperature range, thus,

$$\varepsilon^{\mathrm{rat}} = \int_{T^{\mathrm{crit}}}^{\infty} \phi^{\mathrm{rat}} d\tau \qquad (36)$$

where τ is a dummy variable used to represent temperature. Ratchet growth is assumed to occur when the temperature is increasing and above T^{crit}. The function $\varepsilon^{\max}$ represents the maximum ratchet growth that can be obtained by cycling between T^{crit} and a given temperature τ, and $\phi^{\max}$ is its derivative with respect to the given temperature,

$$\phi^{\max} = \frac{d\varepsilon^{\max}}{d\tau} \qquad (37)$$

Each time the temperature is above T^{crit}, and passes a given temperature on an up cycle, the corresponding value of ϕ^{rat} is incremented a fraction of the way to its asymptotic value. The change in $\phi^{\max}$ is calculated using the closing fraction, z_1. This produces an exponential approach, if cycling between any two temperatures. The ratchet strain is not allowed to ratchet down, thus,

$$\Delta\phi^{\mathrm{rat}} = \max\begin{Bmatrix} z_1 \;\; w \;\; 1+\psi \;\; \phi^{\max} - \phi^{\mathrm{rat}} \\ 0 \end{Bmatrix} \qquad (38)$$

where ψ is a function that enhances the ratchet growth depending on the cold history, and w is a function that suppresses it depending on the current pressure. The value of w ranges between zero and one and ψ is always positive.

$$\psi = z_2 \;\; T^{\mathrm{cut}} - \psi^{\mathrm{cold}} \;\; {}^{z_3} \qquad (39)$$

The value of ψ^{cold} is the lower of T^{cut} or the coldest temperature that the material has seen since it was last at the given temperature. The sensitivity to cold cycles is determined by the constants z_2 and z_3. Figure 11 shows a ratchet response (linear strain) for a data set [2] that may be used to calibrate the constants z_1, z_2 and z_3. Figure 12 show the corresponding temperature history . Note the model deviates from the data when the cold cycle is -130°C, which is colder than our temperature range of interest.

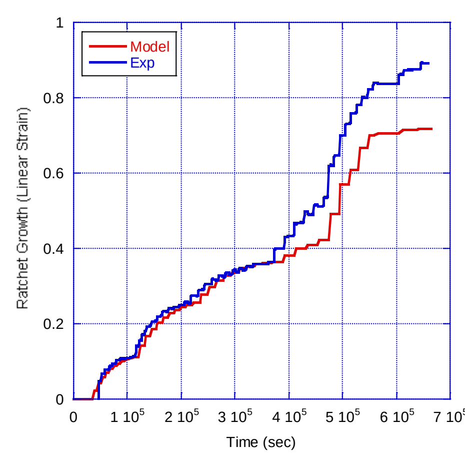

Fig. 11. Comparison Between Ratchet Growth in Experiment and Model.

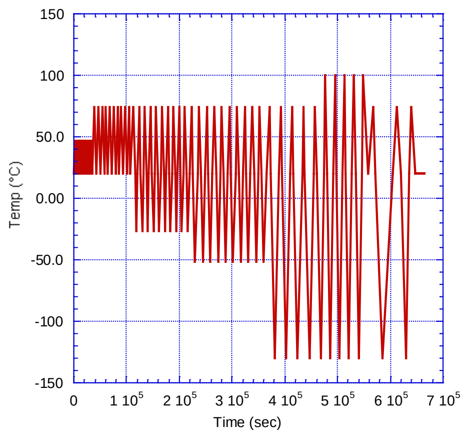

Fig. 12. Temperature History for Ratchet Growth Comparison

Ratchet growth is often an anisotropic phenomenon. This is captured with an anisotropic ratchet growth coefficient, C_{ij}^{rat}

$$\varepsilon_{ij}^{rat} = C_{ij}^{rat}\varepsilon^{rat} \qquad (40)$$

The value C_{ij}^{rat} must be equal to one, in order for it not to change the volumetric ratchet growth. Functions of temperature are discretized into evenly spaced arrays. Linear shape functions are assumed and values are updated accordingly

Putting it all together

In order to find the total deformation each of the strain components must be summed. However, because both the recoverable and non-recoverable strains were formulated to creep at the log-slope of a given material, when both are added directly together, the creep will be overstated. By adding a volume fraction of each creep formulation, in series, the proper behavior is preserved.

$$\varepsilon_{ij} = \varepsilon_{ij}^{Ed} + \mu\varepsilon_{ij}^{rd} + (1-\mu)\varepsilon_{ij}^{nd} + \varepsilon_{ij}^{therm} + \varepsilon_{ij}^{rat} + \frac{(\varepsilon^{Ev} + \mu\varepsilon^{rv} + (1-\mu)\varepsilon^{nv})\delta_{ij}}{3} \qquad (41)$$

The parameter μ represents the volume fraction of the recoverable creep formulation. This parameter essentially determines how much the material will rebound when unloaded. The value of mu is typically around one half. Figure 12 shows the model response to a uniform load followed by its removal at about 170 hours. Figure 14 shows the creep response to a load that is cycled on and off in a square wave.

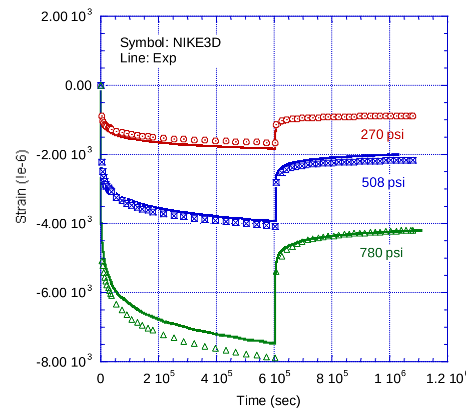

Fig. 13. Numerical and Experimental Creep and Recovery Data.

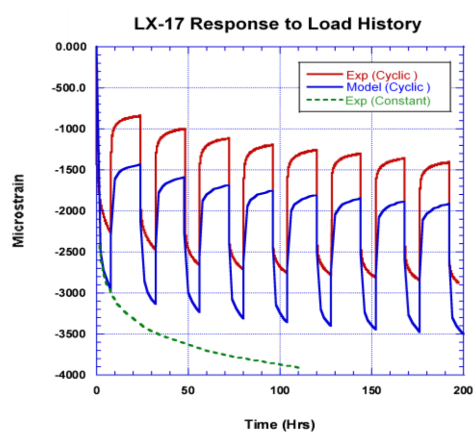

Fig. 14. Numerical and Experimental Creep Response to a Cyclic Square Wave at 500psi and 20°C

Summary

In summary we develop in this paper a comprehensive long time duration model for IHE's and show experimental validation for a variety of creep behaviors including cyclic loading, hydrostatic loading, uni-axial loading, and creep where the third principle stress is varied independently from the first two. Creep at various temperatures is also considered. The strain response of this model is independent of time step size, provided the stress and temperature remain constant. This model has been formulated in three dimensions and implemented in NIKE3D for use in large scale analyses.

References

[1] Puso, M.A. "NIKE3D: A Nonlinear, Implicit, Three-Dimensional Finite Element Code For Solid And Structural Mechanics User's Manual", UCRL-SM-236081, 2007.

[2] Cady, H.H. "Thermal Expansion and Permanent Growth in PBX 9502", 1998

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.